

Triethanolamine
102-71-6 | DTXSID9021392

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 9.22e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.89e-01

Confidence level: 3.97e-01

Nearest Neighbors from the Training Set

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Triallylamine

Measured: 3.59e-06

Predicted: 2.91

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Sulfuramid

Measured: 3.36e-03

Predicted: 4.42e-06

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Heptanedioic acid

Measured: 2.80e-04

Predicted: 1.02e-07

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Glycerol

Measured: 1.68e-04

Predicted: 1.31e-04

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Ethanediamide

Measured: 4.64e-07

Predicted: 7.36e-08